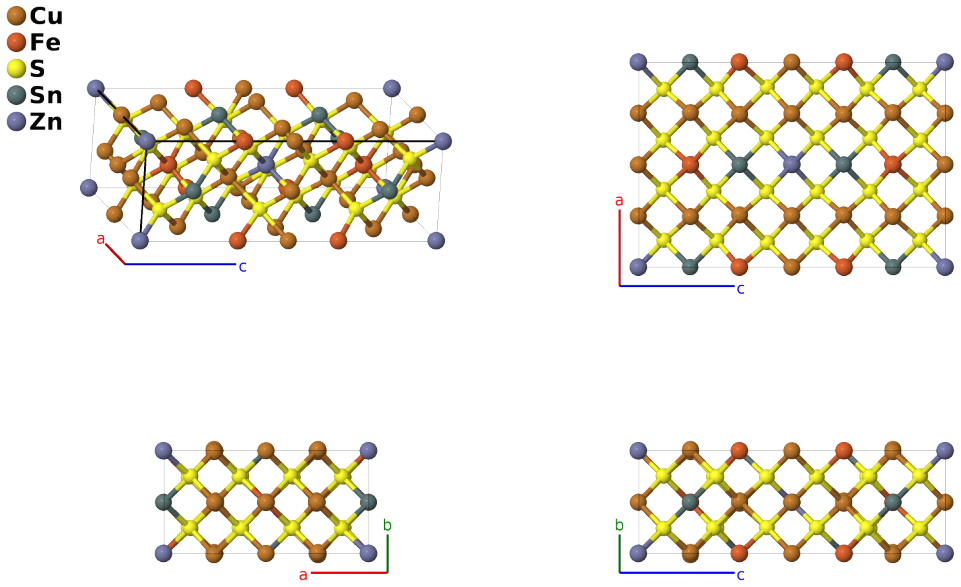
Stannoidite ($Cu_8(Fe,Zn)_3Sn_2S_{12}$) Structure: A8B2C12D2E_oI50_23_acgk_e_3k_f_b-001

This structure originally had the label `A8B2C12D2E_oI50_23_bcfk_i_3k_j_a`. Calls to that address will be redirected here.

Cite this page as: D. Hicks, M. J. Mehl, E. Gossett, C. Toher, O. Levy, R. M. Hanson, G. Hart, and S. Curtarolo, *The AFLOW Library of Crystallographic Prototypes: Part 2*, Comput. Mater. Sci. **161**, S1 (2019). doi: 10.1016/j.commatsci.2018.10.043

https://aflow.org/p/7NS2

https://aflow.org/p/A8B2C12D2E_oI50_23_acgk_e_3k_f_b-001

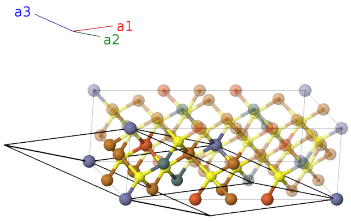


Prototype	$Cu_8Fe_2S_{12}Sn_2Zn$
AFLOW prototype label	A8B2C12D2E_oI50_23_acgk_e_3k_f_b-001
Mineral name	stannoidite
ICSD	41894
Pearson symbol	oI50
Space group number	23
Space group symbol	$I222$
AFLOW prototype command	`aflow --proto=A8B2C12D2E_oI50_23_acgk_e_3k_f_b-001 --params=`$a, b/a, c/a, x_4, x_5, y_6, x_7, y_7, z_7, x_8, y_8, z_8, x_9, y_9, z_9, x_{10}, y_{10}, z_{10}$

- The composition of the Zn (2a) site is actually $Zn_{0.85}Fe_{0.15}$. Here we assume that it is purely zinc.

Body-centered Orthorhombic primitive vectors

$$\mathbf{a_1} = -\tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}b\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_2} = \tfrac{1}{2}a\,\hat{\mathbf{x}} - \tfrac{1}{2}b\,\hat{\mathbf{y}} + \tfrac{1}{2}c\,\hat{\mathbf{z}}$$
$$\mathbf{a_3} = \tfrac{1}{2}a\,\hat{\mathbf{x}} + \tfrac{1}{2}b\,\hat{\mathbf{y}} - \tfrac{1}{2}c\,\hat{\mathbf{z}}$$



Basis vectors

		Lattice coordinates		Cartesian coordinates	Wyckoff position	Atom type
$\mathbf{B_1}$	=	0	=	0	(2a)	Cu I
$\mathbf{B_2}$	=	$\frac{1}{2}\,\mathbf{a}_2 + \frac{1}{2}\,\mathbf{a}_3$	=	$\frac{1}{2}a\,\hat{\mathbf{x}}$	(2b)	Zn I
$\mathbf{B_3}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \frac{1}{2}\,\mathbf{a}_2$	=	$\frac{1}{2}c\,\hat{\mathbf{z}}$	(2c)	Cu II
$\mathbf{B_4}$	=	$x_4\,\mathbf{a}_2 + x_4\,\mathbf{a}_3$	=	$ax_4\,\hat{\mathbf{x}}$	(4e)	Fe I
$\mathbf{B_5}$	=	$-x_4\,\mathbf{a}_2 - x_4\,\mathbf{a}_3$	=	$-ax_4\,\hat{\mathbf{x}}$	(4e)	Fe I
$\mathbf{B_6}$	=	$\frac{1}{2}\,\mathbf{a}_1 + \left(x_5 + \frac{1}{2}\right)\,\mathbf{a}_2 + x_5\,\mathbf{a}_3$	=	$ax_5\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4f)	Sn I
$\mathbf{B_7}$	=	$\frac{1}{2}\,\mathbf{a}_1 - \left(x_5 - \frac{1}{2}\right)\,\mathbf{a}_2 - x_5\,\mathbf{a}_3$	=	$-ax_5\,\hat{\mathbf{x}} + \frac{1}{2}c\,\hat{\mathbf{z}}$	(4f)	Sn I
$\mathbf{B_8}$	=	$y_6\,\mathbf{a}_1 + y_6\,\mathbf{a}_3$	=	$by_6\,\hat{\mathbf{y}}$	(4g)	Cu III
$\mathbf{B_9}$	=	$-y_6\,\mathbf{a}_1 - y_6\,\mathbf{a}_3$	=	$-by_6\,\hat{\mathbf{y}}$	(4g)	Cu III
$\mathbf{B_{10}}$	=	$(y_7 + z_7)\,\mathbf{a}_1 + (x_7 + z_7)\,\mathbf{a}_2 + (x_7 + y_7)\,\mathbf{a}_3$	=	$ax_7\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(8k)	Cu IV
$\mathbf{B_{11}}$	=	$-(y_7 - z_7)\,\mathbf{a}_1 - (x_7 - z_7)\,\mathbf{a}_2 - (x_7 + y_7)\,\mathbf{a}_3$	=	$-ax_7\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} + cz_7\,\hat{\mathbf{z}}$	(8k)	Cu IV
$\mathbf{B_{12}}$	=	$(y_7 - z_7)\,\mathbf{a}_1 - (x_7 + z_7)\,\mathbf{a}_2 - (x_7 - y_7)\,\mathbf{a}_3$	=	$-ax_7\,\hat{\mathbf{x}} + by_7\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}}$	(8k)	Cu IV
$\mathbf{B_{13}}$	=	$-(y_7 + z_7)\,\mathbf{a}_1 + (x_7 - z_7)\,\mathbf{a}_2 + (x_7 - y_7)\,\mathbf{a}_3$	=	$ax_7\,\hat{\mathbf{x}} - by_7\,\hat{\mathbf{y}} - cz_7\,\hat{\mathbf{z}}$	(8k)	Cu IV
$\mathbf{B_{14}}$	=	$(y_8 + z_8)\,\mathbf{a}_1 + (x_8 + z_8)\,\mathbf{a}_2 + (x_8 + y_8)\,\mathbf{a}_3$	=	$ax_8\,\hat{\mathbf{x}} + by_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$	(8k)	S I
$\mathbf{B_{15}}$	=	$-(y_8 - z_8)\,\mathbf{a}_1 - (x_8 - z_8)\,\mathbf{a}_2 - (x_8 + y_8)\,\mathbf{a}_3$	=	$-ax_8\,\hat{\mathbf{x}} - by_8\,\hat{\mathbf{y}} + cz_8\,\hat{\mathbf{z}}$	(8k)	S I
$\mathbf{B_{16}}$	=	$(y_8 - z_8)\,\mathbf{a}_1 - (x_8 + z_8)\,\mathbf{a}_2 - (x_8 - y_8)\,\mathbf{a}_3$	=	$-ax_8\,\hat{\mathbf{x}} + by_8\,\hat{\mathbf{y}} - cz_8\,\hat{\mathbf{z}}$	(8k)	S I
$\mathbf{B_{17}}$	=	$-(y_8 + z_8)\,\mathbf{a}_1 + (x_8 - z_8)\,\mathbf{a}_2 + (x_8 - y_8)\,\mathbf{a}_3$	=	$ax_8\,\hat{\mathbf{x}} - by_8\,\hat{\mathbf{y}} - cz_8\,\hat{\mathbf{z}}$	(8k)	S I
$\mathbf{B_{18}}$	=	$(y_9 + z_9)\,\mathbf{a}_1 + (x_9 + z_9)\,\mathbf{a}_2 + (x_9 + y_9)\,\mathbf{a}_3$	=	$ax_9\,\hat{\mathbf{x}} + by_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}}$	(8k)	S II
$\mathbf{B_{19}}$	=	$-(y_9 - z_9)\,\mathbf{a}_1 - (x_9 - z_9)\,\mathbf{a}_2 - (x_9 + y_9)\,\mathbf{a}_3$	=	$-ax_9\,\hat{\mathbf{x}} - by_9\,\hat{\mathbf{y}} + cz_9\,\hat{\mathbf{z}}$	(8k)	S II
$\mathbf{B_{20}}$	=	$(y_9 - z_9)\,\mathbf{a}_1 - (x_9 + z_9)\,\mathbf{a}_2 - (x_9 - y_9)\,\mathbf{a}_3$	=	$-ax_9\,\hat{\mathbf{x}} + by_9\,\hat{\mathbf{y}} - cz_9\,\hat{\mathbf{z}}$	(8k)	S II
$\mathbf{B_{21}}$	=	$-(y_9 + z_9)\,\mathbf{a}_1 + (x_9 - z_9)\,\mathbf{a}_2 + (x_9 - y_9)\,\mathbf{a}_3$	=	$ax_9\,\hat{\mathbf{x}} - by_9\,\hat{\mathbf{y}} - cz_9\,\hat{\mathbf{z}}$	(8k)	S II
$\mathbf{B_{22}}$	=	$(y_{10} + z_{10})\,\mathbf{a}_1 + (x_{10} + z_{10})\,\mathbf{a}_2 + (x_{10} + y_{10})\,\mathbf{a}_3$	=	$ax_{10}\,\hat{\mathbf{x}} + by_{10}\,\hat{\mathbf{y}} + cz_{10}\,\hat{\mathbf{z}}$	(8k)	S III

$\mathbf{B_{23}}$	=	$-(y_{10}-z_{10})\,\mathbf{a}_1 - (x_{10}-z_{10})\,\mathbf{a}_2 - (x_{10}+y_{10})\,\mathbf{a}_3$	=	$-ax_{10}\,\hat{\mathbf{x}} - by_{10}\,\hat{\mathbf{y}} + cz_{10}\,\hat{\mathbf{z}}$	(8k)	S III
$\mathbf{B_{24}}$	=	$(y_{10}-z_{10})\,\mathbf{a}_1 - (x_{10}+z_{10})\,\mathbf{a}_2 - (x_{10}-y_{10})\,\mathbf{a}_3$	=	$-ax_{10}\,\hat{\mathbf{x}} + by_{10}\,\hat{\mathbf{y}} - cz_{10}\,\hat{\mathbf{z}}$	(8k)	S III
$\mathbf{B_{25}}$	=	$-(y_{10}+z_{10})\,\mathbf{a}_1 + (x_{10}-z_{10})\,\mathbf{a}_2 + (x_{10}-y_{10})\,\mathbf{a}_3$	=	$ax_{10}\,\hat{\mathbf{x}} - by_{10}\,\hat{\mathbf{y}} - cz_{10}\,\hat{\mathbf{z}}$	(8k)	S III

References

[1] Y. Kudoh and Y. Takéuchi, *The superstructure of stannoidite*, Z. Kristallogr. **144**, 145–160 (1976), doi:10.1524/zkri.1976.144.16.145.

Found in

[1] R. T. Downs and M. Hall-Wallace, *The American Mineralogist Crystal Structure Database*, Am. Mineral. **88**, 247–250 (2003).